Optimization notes

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Directional derivative

From a starting point $\underline{x}_0$ and a given dirction $\underline{u}$:

- $\underline{x}(\lambda) = \underline{x}_0 + \lambda \underline{u}$
  - λ is a scalar.
- $d\underline{x} = \underline{u} d\lambda$
  - For a small change in λ.
- $F(\lambda) = f(\underline{x}_0 + \lambda \underline{u})$

$$
\begin{aligned}
dF = df &= (\nabla f(\underline{x}))^\top d\underline{x} \\
&= (\nabla f(\underline{x}))^\top \underline{u} d\lambda = \nabla^\top f \underline{u} \lambda
\end{aligned}
$$

- $\frac{df}{d\lambda} = \nabla^\top f \underline{u}$
  - If f is minimized at $\underline{x}^* = \underline{x}_0 + \lambda \underline{u}$, then:
    - $\nabla f(\underline{x}^*))^\top f \underline{u} = 0$
    - gradient f evaluated at the minimum point is orthogonalto $\underline{u}$.

Weierstrass Theorem

If $f(\underline{x})$ is continuous on a nonempty feasible set that is cloased and bounded, then $f(\underline{x})$ has a global minimum in this set.

- A set S is bounded if for any point $\underline{x}$ in S, we have $\underline{x}^\top \underline{x} < c$
  - c is a finite positive number.

Single-variable unconstrained optimization

- Necessary condition
  - If a function $f(x)$ has a local minimum at $x = x^*$, and $f'(x)$ exists as a finite number at $x = x^*$, then $f'(x^*) = 0$.
  - x^* at $f'(x^*) = 0$ is called stationary point.
- Sufficient condition
  - Suppose $f'(x^*) = f''(x^*) = \cdots = f^{(m-1)}(x^*) = 0$, but $f^{(m)}(x^*) \neq 0$, then $f(x^*)$ is:
    - 1. a local minimum if $f^{(m-1)}(x^*) > 0$ and m is even.
    - 2. a local maximum if $f^{(m-1)}(x^*) < 0$ and m is even.
    - 3. neither a maximum nor a minimum if m is odd.

Multi-variable unconstrained optimization (1)

Definition of r^{th} differential of function f:

$$d^r f(\underline{x}^*) = \sum_{i=1}^{n} \sum_{j=1}^{n} \cdots \sum_{k=1}^{n} h_i h_j \ldots h_k \frac{\partial^r f(\underline{x}^*)}{\partial x_i \partial x_j \ldots \partial x_k}$$

Example

When (order) $r = 2$ and (number of variables) $n = 3$, we have:

$$\begin{aligned} d^2 f(\underline{x}^*) = d^2 f(x_1^*, x_2^*, x_3^*) &= \sum_{i=1}^{3} \sum_{j=1}^{3} h_i h_j \frac{\partial^2 f(\underline{x}^*)}{\partial x_i \partial x_j} \\ &= h_1^2 \frac{\partial^2 f(\underline{x}^*)}{\partial x_1^2} + h_2^2 \frac{\partial^2 f(\underline{x}^*)}{\partial x_2^2} + h_3^2 \frac{\partial^2 f(\underline{x}^*)}{\partial x_3^2} \\ &+ 2h_1 h_2 \frac{\partial^2 f(\underline{x}^*)}{\partial x_1 \partial x_2} + 2h_2 h_3 \frac{\partial^2 f(\underline{x}^*)}{\partial x_2 \partial x_3} + 2h_1 h_3 \frac{\partial^2 f(\underline{x}^*)}{\partial x_1 \partial x_3} \end{aligned}$$

Multi-variable unconstrained optimization (2)

- Necessary condition

$$\frac{\partial f(\underline{x}^*)}{\partial x_1} = \frac{\partial f(\underline{x}^*)}{\partial x_2} = \cdots = \frac{\partial f(\underline{x}^*)}{\partial x_n} = 0$$

  - In vector form, $\nabla f(\underline{x}^* = 0)$.
  - $\underline{x}^*$ at $\nabla f(\underline{x}^* = 0)$ is called stationary point.
- Sufficient condition
  - For a stationary point at $\underline{x} = \underline{x}^*$:
    - if the Hessian matrix of $f(\underline{x})$ evaluated at $\underline{x} = \underline{x}^*$ is positive definite, then $\underline{x}^*$ is a local minimum.
    - if the Hessian matrix of $f(\underline{x})$ evaluated at $\underline{x} = \underline{x}^*$ is negative definite, then $\underline{x}^*$ is a local maximum.

Hessian Matrix

- $(H_f)_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_n}$
- In matrix form: $H_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$

Definiteness

- A matrix is positive definite if all its eigenvalues are positive.
  - If some of the eigenvalues are positive and some are zero, then the matrix is positive semidefinite.
- Checking the sign of the determinants is an alternative way to determine the definiteness of a matrix.
- A twice differentiable function is convex if and only if its Hessian matrix is positive semi-definite.
  - The function is strictly convex if the Hessian matrix is positive definite.

Multivariable optimization with equality constraints

Lagrange Multiplier Theorem

- Suppose the point $\underline{x}^*$ minimizes $f(\underline{x})$ and satisfies the equality constraints: $h_j(\underline{x}^*) = 0$, for $j = 1, 2, \ldots, m$
- Assume that the constraint gradients $\nabla h_j(\underline{x}^*)$ are linealy independent.
- Then there exists a unique set λ_j^* $(j = 1, 2, \ldots, m)$ satisfying:

$$\frac{\partial L}{\partial x_i} = \frac{\partial f}{\partial x_i} + \sum_{j=1}^{m} \lambda_j^* \frac{\partial h_j}{\partial x_i} = 0$$

where $i = 1, 2, \ldots, n$.

Simplex method (Non-linear programming)

Definition of Simplex

The geometric figure formed by a set of n + 1 points in an n-dimensional space is called a simplex.

- When the points are equidistant, the simplex is said to be *regular*.
- In two dimensions the simplex is a triangle, and in three dimensions, it is a tetrahedron.
- The simplex method was originally given by Spendley et al. and was developed later by Nelder and Mead.

Simplex method: Steps

Choose a reflection coefficient $\alpha > 0$, an expansion coefficient $\gamma > 1$, and a contraction coefficient $0 < \beta < 1$.

1. Identify $\underline{x}_{\text{min}}$ and $\underline{x}_{\text{max}}$ amoung $\{\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_{n+1}\}$
   - such that $f(\underline{x}_{\text{min}})$ is the minimum and $f(\underline{x}_{\text{max}})$ is the maximum of all the $f(\underline{x}_i)$, for $i = 1, 2, \ldots, n+1$.
   - If $|\underline{x}_{\text{max}} - \underline{x}_{\text{min}}| < \epsilon$, stop. The minimum is at $\underline{x}_{\text{min}}$.
   - Otherwise, let $\underline{x}_a$ be the averaged position of $\{x_1, x_2, \ldots, x_{n+1}\}$, **excluding** $\underline{x}_{\text{max}}$, and go to step 2.
2. Let the reflection point $\underline{x}_r = \underline{x}_a + \alpha(\underline{x}_a - \underline{x}_{\text{max}})$.
   - If $f(\underline{x}_{min}) > f(\underline{x}_r)$, let the expansion point $\underline{x}_e = \underline{x}_a + \gamma(\underline{x}_r - \underline{x}_a)$, and go to step 3.
   - Otherwise, go to step 4.

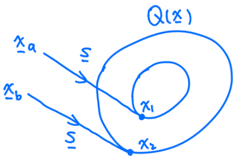
Simplex method: Steps

3. If $f(\underline{x}_r) > f(\underline{x}_e)$, the point $\underline{x}_{\max}$ is replaced by $\underline{x}_e$.
   - Otherwise, $\underline{x}_{\max}$ is replaced by $\underline{x}_r$. A new set of n+1 points is formed. Then go to step 1.
4. If the second largest $f(\underline{x}_i) > f(\underline{x}_r)$, then $\underline{x}_{\max}$ is replaced by $\underline{x}_r$ to form a new set of n+1 points, and go to step 1.
   - Otherwise, go to step 5.
5. Let $\underline{x}_p$ be defined such that $f(\underline{x}_p) = \min\{f(\underline{x}_r), f(\underline{x}_{\max})\}$ and let the contraction point $\underline{x}_c = \underline{x}_a + \beta(\underline{x}_p - \underline{x}_a)$.
   - If $f(\underline{x}_c) > f(\underline{x}_p)$, replace $\underline{x}_j$ by $\underline{x}_j + (\underline{x}_{\min} - \underline{x}_j)/2$, for $j = 1, 2, \ldots, n+1$, and go to step 1.
   - Otherwise, $\underline{x}_c$ replaces $\underline{x}_{\max}$ to form a new set of n+1 points, and go to step 1.

Quadratic function

$$Q(\underline{x}) = \frac{1}{2}\underline{x}^\top A\underline{x} + B^\top\underline{x} + C$$

From the two starting points x_a and x_b, function minimum is searched along the same direction $\underline{S}$, reaching the minimum points $\underline{x}_1$ and $\underline{x}_2$, respectively.



Then $\underline{S}^T A(x_1 - x_2) = 0$

Then the line joining x_1 and x_2 is A-conjugate to $\underline{S}$.
$\Rightarrow S_i^\top A S_j^\top \neq 0$, for $i \neq j$. $(i = 1, 2, \ldots, n; j = 1, 2, \ldots, n)$

Conjugate gradient method

During the $(j+1)^{th}$ saerch from point $\underline{x}_{j+1}$, the search direction is given by:

$$\underline{S}_{j+1} = -\nabla f(\underline{x}_{j+1}) + \beta_j \underline{S}_j$$

where

$$\beta_j = \frac{\nabla f_{j+1}^{\top} \nabla f_{j+1}}{\nabla f_j^{\top} \nabla f_j}$$

Conjugate gradient method (Proof - 1)

From Quadratic function:

$$f(\underline{\mathrm{x}}) = \frac{1}{2}\underline{\mathrm{x}}^{\top}\mathrm{A}\underline{\mathrm{x}} + \mathrm{B}^{\top}\underline{\mathrm{x}} + \mathrm{C}$$
$$f'(\underline{\mathrm{x}}) = \mathrm{A}\underline{\mathrm{x}} + \mathrm{B}$$

From steepest descent direction with step length λ:

$$\underline{x}_2 = \underline{x}_1 + \lambda_1^* \underline{S}_1$$

Conjugate gradient method (Proof - 2)

Minimize f to obtain the optimized λ^*:

$$
\begin{aligned}
\frac{df}{d\lambda_1^*} &= \sum_{i=1}^{n} \frac{\partial f}{\partial (x_1 + \lambda_1^* S_1)} \frac{\partial (x_1 + \lambda_1^* S_1)}{\partial \lambda_1^*} \\
&= \nabla f(x_1 + \lambda_1^* S_1)^\top \cdot S_1 \\
&= [\mathrm{A}(x_1 + \lambda_1^* S_1) + \mathrm{B}]^\top \cdot S_1 \\
&= [\mathrm{A}x_1 + \mathrm{B} + \mathrm{A}\lambda_1^* S_1]^\top \cdot S_1 \\
&= [\nabla f_1 + \mathrm{A}\lambda_1^* S_1]^\top \cdot S_1 \\
&= \nabla f_1^\top S_1 + \lambda_1^* S_1^\top \mathrm{A} S_1 = 0
\end{aligned}
$$

Thus, we can get $\lambda_1^* = -\frac{\nabla f_1^\top S_1}{S_1^\top \mathrm{A} S_1}$

Conjugate gradient method (Proof - 3)

From steepest descent direction with step length λ:

$$x_2 = x_1 + \lambda_1^* S_1$$

$$\Rightarrow \frac{1}{\lambda_1^*}(x_2 - x_1) = S_1$$

Multipliy A and change left and right side:

$$\Rightarrow \mathrm{A} S_1 = \frac{1}{\lambda_1^*}\mathrm{A}(x_2 - x_1)$$

$$\Rightarrow S_2^\top \mathrm{A} S_1 = \frac{1}{\lambda_1^*} S_2^\top \mathrm{A}(x_2 - x_1) = 0$$

Currently, we know $\frac{1}{\lambda_1^*}$ is not zero. $\Rightarrow S_2^\top \mathrm{A}(x_2 - x_1) = 0$

Conjugate gradient method (Proof - 4)

$$
\begin{aligned}
S_2^\top \mathrm{A}(x_2 - x_1) &= S_2^\top(\mathrm{A}x_2 + \mathrm{B} - \mathrm{A}x_1 - \mathrm{B}) \\
&= S_2^\top(\nabla f_2 - \nabla f_1) \\
&= (-\nabla f_2 + \beta_2 S_1)^\top(\nabla f_2 - \nabla f_1) \\
&= -\nabla f_2^\top \nabla f_2 + {\color{red}\nabla f_2^\top \nabla f_1} - {\color{red}\beta_2 \nabla f_1^\top \nabla f_2} + \beta_2 \nabla f_1^\top \nabla f_1
\end{aligned}
$$

$$
\nabla f_2 = \nabla f_1 + \mathrm{A}\lambda_1^* S_1 = \nabla f_1 - \lambda_1^* \mathrm{A} \nabla f_1
$$

$$
\begin{aligned}
\nabla f_2^\top \nabla f_1 &= (\nabla f_1 - \lambda_1^* \mathrm{A} \nabla f_1)^\top \nabla f_1 \\
&= (\nabla f_1 + \frac{\nabla f_1^\top S_1}{S_1^\top \mathrm{A} S_1} \mathrm{A} \nabla f_1)^\top \nabla f_1 \\
&= (\nabla f_1 - \frac{\nabla f_1^\top \nabla f_1}{\nabla f_1^\top \mathrm{A} \nabla f_1} \mathrm{A} \nabla f_1)^\top \nabla f_1 = 0 \cdot \nabla f_1 = 0
\end{aligned}
$$

Conjugate gradient method (Proof - 5)

Because $\nabla f_2^\top \nabla f_1 = 0$

$$\Rightarrow S_2^\top \mathrm{A}(x_2 - x_1) = -\nabla f_2^\top \nabla f_2 + \beta_2 \nabla f_1^\top \nabla f_1 = 0$$

$$\Rightarrow \beta_2 = \frac{\nabla f_2^\top \nabla f_2}{\nabla f_1^\top \nabla f_1}$$

Transformation techniques

It may be possible to convert a constrained optimization problem into an unconstrained one by making a change of variables.
If lower and upper bounds on x_i are specified as:

$$l_i \leq x_i \leq u_i$$

which can be satisfied by transforming the variable x_i as:

$$x_i = l_i + (u_i - l_i) \sin^2 y_i$$

where y_i is the new variable, which can take any value.

- If x_i is restricted to lie in the interval $(0, 1)$, $x_i = \sin^2 y$

Transformation techniques

1. The constraints $g_i(\mathrm{X})$ must be very simple.
2. For certain constraints, it may not be possible to find the necessary transformation.
3. If it is not possible to eliminate all the constraints by making a change of variables.
   - It may be better not to use the transformation at all.
   - However, the partial transformation may sometimes produce a distorted objective function which might be harder to minimize than the original function.

Penalty function method

Find X which minimizes $f(\mathrm{X})$ is converted into an unconstrained minimization problem by constructing a function of the form:

$$\phi_k = \phi(\mathrm{X}, r_k) = f(\mathrm{X}) + r_k \sum_{j-1}^{m} G_j[g_j(\mathrm{X})]$$

- g_j: inequality constraints
- G_j: some function of the constraint g_j
- r_k: penalty parameter (a positive constant)
- $r_k \sum_{j-1}^{m} G_j[g_j(\mathrm{X})]$ is the penalty term.

Interior and exterior penalty function method

- Interior method:

$$G_j = -\frac{1}{g_j(\mathrm{X})}$$

or

$$G_j = -\log[-g_j(\mathrm{X})]$$

- Exterior method:

$$G_j = \max[0, g(\mathrm{X})]$$

or

$$G_j = \{\max[0, g(\mathrm{X})]\}^2$$